Amiloride

2609-46-3 | DTXSID9043853

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 174 °C

Global applicability domain: Outside

Local applicability domain index: 1.76e-01

Confidence level: 6.90e-01

Nearest Neighbors from the Training Set

Image not found
Hexamethylolmelamine
Measured: 137
Predicted: 141

Image not found
Famotidine
Measured: 164
Predicted: 171

Image not found
L-Canavanine
Measured: 184
Predicted: 182

Image not found
Sulfaguanidine
Measured: 192
Predicted: 189